

Spinon-Holon Recombination in Gutzwiller Projected Wave Functions

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The Gutzwiller projection is shown to induce nontrivial correlation between the spinon and the holon in the slave Boson theory of the $t - J$ model. We find this correlation is responsible for some subtle differences between the slave Boson mean field theory and the Gutzwiller projected wave function (GWF), among which the particle-hole asymmetry in the quasiparticle weight calculated from the GWF is a particular example.

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Superconductivity results from Bose condensation of charged particles. In the BCS theory of superconductivity, Fermionic electrons are paired into Bosonic Cooper pairs which then condense into a superfluid. Soon after the discovery of high temperature superconductors, Anderson proposed an exotic way toward superconductivity in this class of materials. Anderson's proposal for superconductivity is to fractionalize the electron, rather than pair them up [1, 2, 3]. According to Anderson's argument, doping holes into the parent compounds of the high temperature superconductors, which are two dimensional antiferromagnetic insulators, would generate a liquid-type spin state called RVB state. Anderson argued that the excitations above the RVB state are fractionalized. More specifically, the spin and the charge quantum number of the electron are carried separately by two kinds of excitations, namely a spin- $\frac{1}{2}$ Fermionic excitation called spinon and a charge 1 Bosonic charged excitation called holon. In such a spin-charge separated system, the charged holon is liberated from the Fermionic statistics of the electron and is ready to condense into a superfluid.

A problem with Anderson's proposal is that the predicted T_c is too high [4, 5]. The holon supercurrent is not efficiently dissipated in this mechanism. In the BCS theory of superconductivity, the supercurrent is dissipated by thermally generated quasiparticle excitations. These quasiparticles, which are charged Fermionic excitations, form a normal fluid and cause dissipative response in external electromagnetic (EM) field. On the other hand, in an ideal spin-charge separated system, the Fermionic spinon has been deprived of the charge to cause dissipative response in an EM field, while the Bosonic excitation of the holon system is very inefficient in dissipating the supercurrent.

One suggested solution for the above problem is to recombine the separated spinon and holon [6, 7, 8]. By spinon-holon recombination, the Fermionic spinon excitation acquires the charge to cause dissipation in an EM field, or, the charged holon regains the Fermionic statis-

tics to be transformed into a normal carrier outside the condensate.

However, the origin and even the exact meaning of such recombination are still elusive. In this paper, we address the problem of spinon-holon recombination in the slave Boson theory of the $t - J$ model. The slave Boson theory is the most direct way to realize the RVB idea. In the slave Boson theory, the constrained electron operator $\hat{c}_{i\sigma}$ is rewritten as $f_{i\sigma} b_i^\dagger$, in which $f_{i\sigma}$ denotes the Fermionic spinon and b_i^\dagger denotes the Bosonic holon. To be a faithful representation of the original electron, the slave particles should be subjected to the local constraint $\sum_\sigma f_{i,\sigma}^\dagger f_{i,\sigma} + b_i^\dagger b_i = 1$.

At the mean field level, the local constraint on the slave particle is relaxed to a global one. The spinon and the holon then move independently. Wen and Lee proposed that the Gaussian fluctuation around the mean field solution, which are gauge fluctuations, tends to recombine the spinon and the holon [7]. However, the lack of a reliable treatment of gauge fluctuation in 2+1 dimension makes it hard to make any quantitative prediction.

In this paper, we address the problem of spinon-holon recombination in the Gutzwiller projected wave functions (GWF). The GWF is derived from the slave Boson mean field state by filtering out its unphysical components with doubly occupied sites. Technically, the Gutzwiller projection, which enforces the local constraint, accounts partially for the effect of gauge fluctuation. Thus some kind of spinon-holon recombination is expected in GWF. We find the Gutzwiller projection not only enforces the local constraint, but also induces longer range correlation between the spinon and the holon. This correlation is given by a well defined correlation function and is found to be responsible for some subtle differences between the mean field theory and the GWF. For example, the particle-hole asymmetry in the quasiparticle weight calculated from GWF is shown to be due to this correlation.

We start from the $t - J$ model which is defined as

$$H = -t \sum_{\langle i,j \rangle, \sigma} (\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + h.c.) + J \sum_{\langle i,j \rangle} (\mathbf{S}_i \mathbf{S}_j - \frac{1}{4} n_i n_j), \quad (1)$$

in which $\mathbf{S}_i = \sum_{\alpha\beta} \hat{c}_{i,\alpha}^\dagger \sigma_{\alpha\beta} \hat{c}_{i,\beta}$ and $n_i = \sum_{\alpha} \hat{c}_{i,\alpha}^\dagger \hat{c}_{i,\alpha}$. The electron operator $\hat{c}_{i,\sigma}$ in (1) is subjected to the constraint of no double occupancy

$$\sum_{\sigma} \hat{c}_{i,\sigma}^\dagger \hat{c}_{i,\sigma} \leq 1. \quad (2)$$

In terms of the spinon and the holon operator, the $t - J$ model reads[4]

$$H = -t \sum_{\langle i,j \rangle, \sigma} (f_{i,\sigma}^\dagger f_{j,\sigma} b_i^\dagger b_i + h.c.) + \frac{J}{2} \sum_{\langle i,j \rangle, \alpha, \beta} (f_{i\alpha}^\dagger f_{i\beta} f_{j\beta}^\dagger f_{j\alpha} - f_{i\alpha}^\dagger f_{i\alpha} f_{j\beta}^\dagger f_{j\beta}),$$

in which $f_{i\alpha}$ and b_i are now subjected to the constraint

$$\sum_{\sigma} f_{i,\sigma}^\dagger f_{i,\sigma} + b_i^\dagger b_i = 1. \quad (3)$$

In the mean field theory, the interaction term is decoupled by introducing RVB order parameter $\chi_{ij} = \sum_{\sigma} \langle f_{i,\sigma}^\dagger f_{j,\sigma} \rangle$ and $\Delta_{ij} = \sum_{\alpha} \langle \epsilon_{\alpha\beta} f_{i,\alpha}^\dagger f_{j,\beta} \rangle$, in which $\epsilon_{\alpha\beta}$ is the total antisymmetric tensor. The local constraint is relaxed to a global one. The mean field Hamiltonian for the spinon and the holon take the form

$$H_f = \sum_{\mathbf{k}, \sigma} \xi_{\mathbf{k}} f_{\mathbf{k},\sigma}^\dagger f_{\mathbf{k},\sigma} + \sum_{\mathbf{k}, \sigma} \Delta_{\mathbf{k}} (f_{\mathbf{k},\sigma}^\dagger f_{-\mathbf{k},\sigma}^\dagger + h.c.) \quad (4)$$

and

$$H_h = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} \quad (5)$$

in momentum space. The mean field ground state is given by the following product

$$|G\rangle_{\text{MF}} = (b_{q=0}^\dagger)^{N_b} |\text{BCS}\rangle, \quad (6)$$

in which $|\text{BCS}\rangle$ denotes the BCS pairing state of the spinon. A mean field excitation, for, say, a hole-like quasiparticle, is given by

$$|\mathbf{k}, \sigma\rangle_{\text{MF}} = b_{q=0}^\dagger \gamma_{\mathbf{k}\sigma}^\dagger |G\rangle_{\text{MF}}, \quad (7)$$

in which $\gamma_{\mathbf{k}\sigma}^\dagger$ denotes the Bogliubov quasiparticle of the BCS Hamiltonian for spinon.

The GWF for the ground state is given by projecting $|G\rangle_{\text{MF}}$ into the subspace that satisfy the constraint Eq.(3),

$$|G\rangle_{\text{Var}} = P_G (b_{q=0}^\dagger)^{N_b} |\text{BCS}\rangle, \quad (8)$$

in which $|G\rangle_{\text{Var}}$ denotes the variational ground state and P_G denotes the Gutzwiller projection. Similarly, $P_G |\mathbf{k}\rangle_{\text{MF}}$ provides a variational guess for the quasiparticle excitation on $|G\rangle_{\text{Var}}$. The same construction for the quasiparticle excitation is used in some recent works[9].

The spinon-holon recombination in GWF can be most easily seen by inspecting the quasiparticle weight $Z_{\mathbf{k}}$. In the mean field theory, $Z_{\mathbf{k}}$ scales linearly with hole density, since the coherent spectral weight is caused by holon condensation. However, $Z_{\mathbf{k}}$ calculated from GWF vanishes more slowly near half filling. For example, $Z_{\mathbf{k}}$ calculated from the one dimensional GWF vanishes as $x^{1/2}$ near half filling[10]. Similar behavior is also observed in two dimensional systems[11]. In some cases, $Z_{\mathbf{k}}$ calculated from GWF can even be nonzero at half filling[12]. This discrepancy can be naturally explained by invoking spinon-holon recombination in GWF.

Now we define spinon-holon recombination in GWF more explicitly. For clarity's sake, we first consider a half filled system and assume the spinon pairing term to be absent[13]. The mean field ground state of the system is then given by a half filled spinon Fermi sea, while a hole-like quasiparticle is generated as follow

$$|\mathbf{k}, \uparrow\rangle_{\text{MF}} = b_{q=0}^\dagger f_{-\mathbf{k}, \downarrow} |\text{FS}\rangle, \quad (9)$$

in which $|\text{FS}\rangle$ denotes the half filled Fermi sea. At the mean field level, $|\mathbf{k}, \uparrow\rangle_{\text{MF}}$ is interpreted as a state with an added holon and a hole of spinon on the background of $|\text{FS}\rangle$. In real space,

$$|\mathbf{k}, \uparrow\rangle_{\text{MF}} = \frac{1}{N} \sum_{i,j} e^{ik(r_i - r_j)} b_i^\dagger f_{j\downarrow} |\text{FS}\rangle. \quad (10)$$

Thus, the added holon and the hole of spinon move independently on $|\text{FS}\rangle$ and have a chance of only $\frac{1}{N}$ to recombine into the original electron. This explains the vanishing of the quasiparticle weight at half filling in the mean field theory.

Now let's see what happens when the local constraint is enforced by the Gutzwiller projection. The projected wave function for the above quasiparticle is given by

$$|\mathbf{k}, \uparrow\rangle_{\text{Var}} = \frac{1}{N} \sum_{i,j} e^{ik(r_i - r_j)} P_G b_i^\dagger f_{j\downarrow} |\text{FS}\rangle. \quad (11)$$

Following the convention of the mean field theory, we interpret the index i and j as the locations of the added holon and the hole of spinon. The difference between $|\mathbf{k}, \uparrow\rangle_{\text{Var}}$ and $|\mathbf{k}, \uparrow\rangle_{\text{MF}}$ can be understood as follows. In the mean field theory, the relative motion between the added holon and the hole of spinon is described by plane wave factor. The background particles in $|\text{FS}\rangle$ do not contribute to their correlation. After the Gutzwiller projection, the added particles get correlated with the background particles through the local constraint. Thus the background particles in $|\text{FS}\rangle$ can also contribute to

the correlation between the added holon and the hole of spinon in $|k, \uparrow\rangle_{\text{Var}}$.

First, we assume $i \neq j$. Due to the local constraint, spinons in $|\text{FS}\rangle$ must keep away from the site i , which is already assigned to the added holon. At the same time, site j should be doubly occupied in $|\text{FS}\rangle$, since it accommodates a spin in the projected state. The sites other than i and j should be all singly occupied in $|\text{FS}\rangle$. Thus, the probability of finding the holon at site i while the hole of spinon at site j , which is denoted as P_{ij} , is given by that of finding site i empty, site j doubly occupied, and all other sites singly occupied in $|\text{FS}\rangle$. For $i = j$, in which case a real electron is removed from site i , the corresponding probability (P_{ii}) is given by that of finding site i occupied by a down spin and all other sites singly occupied in $|\text{FS}\rangle$. The ratio between P_{ij} and P_{ii} is given by

$$\frac{P_{ij}}{P_{ii}} = \frac{\sum_{\beta} |\psi_{\beta}|^2}{\sum_{\alpha} |\psi_{\alpha}|^2} = \frac{\sum_{\alpha} |\psi_{\alpha}|^2 \frac{|\psi_{\beta}|^2}{|\psi_{\alpha}|^2}}{\sum_{\alpha} |\psi_{\alpha}|^2}. \quad (12)$$

Here, ψ_{α} denotes the amplitude of $|\text{FS}\rangle$ for a general configuration $|\alpha\rangle$ in the subspace of no double occupancy, ψ_{β} denotes the amplitude for the configuration derived from $|\alpha\rangle$ by moving an electron (of either spin) from site i to site j . This statistical sum can be evaluated easily with Variational Monte Carlo method.

To see the value of the thus defined correlation function, we consider some special cases in which the effect of spinon-holon recombination is manifest. As a trivial example, we consider the case of removing an electron from a fully polarized spin background. According to the slave Boson mean field theory, the quasiparticle weight is given by the hole density and vanishes at half filling. However, since the spin is fully polarized, the state in consideration is in fact a mean field state in which the quasiparticle weight should be exactly one. This discrepancy can be easily resolved by noting that P_{ij} is nonzero only for $i = j$ on a fully polarized spin background. This indicates that the added holon and the hole of spinon must occupy the same site and thus recombine into a real electron on that site.

As a less trivial example, we consider a state with antiferromagnetic long range order. As we will show below, P_{ij} decays exponentially in this case. The exponential decay of P_{ij} can be understood by noting the opening of a SDW gap between configuration $|\beta\rangle$ and $|\alpha\rangle$ in Eq. (12). Thus the added holon and the hole of spinon will form a well defined bound state in such a spin background. Since the bound state has a nonzero overlap with a bare electron, the quasiparticle weight should be finite even at half filling. Calculation in [12] does find a finite quasiparticle weight for such a state.

Now we present the numerical results. Figure 1 shows the correlation function for the one dimensional projected Fermi sea. The correlation function decays as $1/r$ at large

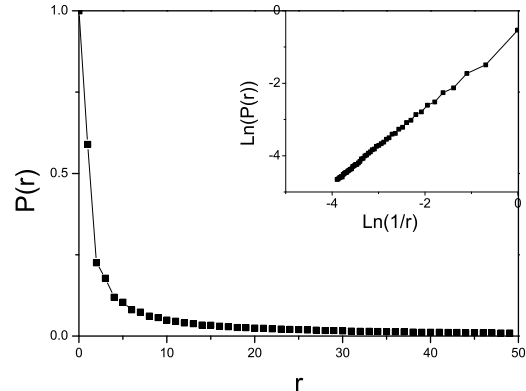


FIG. 1: Spinon - holon correlation function for the one dimensional projected Fermi sea. The inset show the data in logarithmic scale.

distance and is unnormalizable. Thus the quasiparticle weight should vanish at half filling. The result for the two dimensional d-wave RVB state is shown in Figure 2. The correlation function now decays as $1/r^2$ at large distance, which is also unnormalizable. Thus the quasiparticle weight should also vanish at half filling in this state. In Figure 3, we show the result for the antiferromagnetic ordered state. As mentioned above, the correlation function decays exponentially in this case. However, the short range behavior is quite similar to that of the d-wave RVB state.

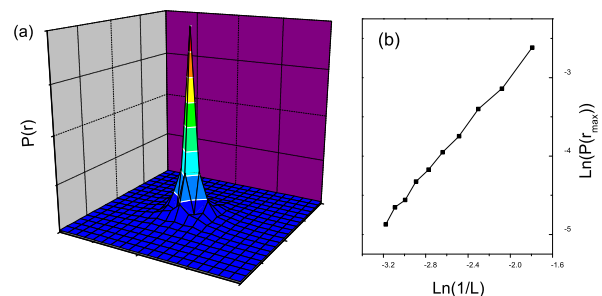


FIG. 2: (a) Spinon - holon correlation function for a d-wave RVB state. The d-wave RVB order parameter $\Delta/t = 0.25$. The calculation is done on a 20×20 lattice. (b) Power law decay of the spinon - holon correlation function. L denotes the linear size of the lattice, r_{max} is largest distance that can be defined on a periodic lattice of size L .

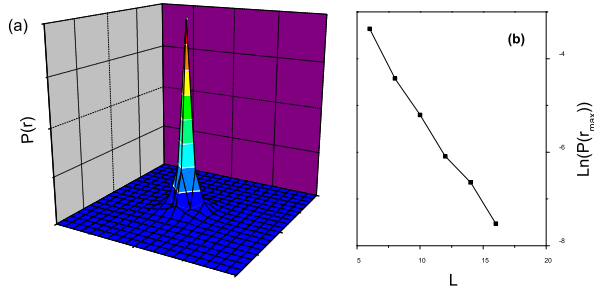


FIG. 3: (a) Same as Figure 2, but now for an antiferromagnetic ordered state. The SDW and d-wave order parameters are $\Delta_{AF}/t = 0.1$ and $\Delta/t = 0.25$. (b) Exponential decay of the spinon - holon correlation function.

The spinon-holon recombination discussed above refers to the correlation between the added particles rather than that between the background particles. At finite doping, a holon condensate is established and the background spinon has a chance of x to behave as a coherent quasiparticle. In fact, the latter is the only way that the system can build a finite quasiparticle weight on the particle side of the spectrum. Following essentially the same steps detailed above, one easily sees that the added slave particles (or hole of them) during the process of injecting an electron have no correlation with each other. Since the quasiparticle weight due to holon condensation is by definition particle-hole symmetric, the particle-hole asymmetry in the quasiparticle weight should be attributed to the spinon-holon recombination effect discussed in this paper[11].

Especially, while the quasiparticle weight for adding an electron is constrained by the sum rule to vanish at half filling, the quasiparticle weight for removing an electron can be finite at half filling, provided that the added holon and the hole of spinon form well defined bound state, as is the case in the antiferromagnetic ordered state. In such a case the quasiparticle can contribute a substantial part of the tunneling asymmetry, although for a full understanding of the latter one also should take into account the contribution from incoherent spectral weight[14]. When the added holon and the hole of spinon are less tightly bounded, the particle-hole asymmetry in the quasiparticle weight should be less dramatic, as is found in a recent work on the tunneling asymmetry of high temperature superconductors[11].

We now discuss some other effects of spinon-holon recombination. By recombining with a spinon excitation, a

hole changes the local spin environment around it. This effect can be invoked to release the kinetic energy of the holes in certain spin background through spontaneous generation of spinon excitations in the system. An example in this respect is provided by a recent variational study on the slightly doped cuprates[12]. In that work, a $t - J$ model with next-nearest-neighboring hopping term is considered. At small doping, it is found that a variational state with spontaneously generated spinon excitations give lower energy than a state without spinon excitations. It is also found that the presence of these spinon excitations changes the charge correlation dramatically. This can also be understood in terms of spinon-holon recombination defined in this paper. A detailed analysis of these issues will appear in separate paper.

Finally, we revisit the problem of supercurrent dissipation. In the presence of spinon excitations, a holon tends to bind with them and form a Fermionic composite object. A holon is thus transformed into a normal charge carrier out of its condensate. The superconductivity is gone when all holons in the condensate are transformed into normal carriers. At low doping, a small number of spinon excitation is enough to kill the superconductivity which is not expected to alter the spin correlation significantly. This is proposed as a mechanism for the pseudogap in underdoped cuprates[6, 7].

In conclusion, an explicit definition for spinon-holon recombination is given on the GWF. The thus defined spinon-holon recombination is shown to be responsible for the particle-hole asymmetry in the quasiparticle weight calculated from the GWF and some other subtle differences between the mean field theory and the GWF. A new mechanism for the dissipation of supercurrent in the RVB state is proposed based on the spinon-holon recombination defined in this paper.

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